

WELLS 09/744,550

=> file hcaplus

FILE 'HCAPLUS' ENTERED AT 17:27:52 ON 21 JUL 2003
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FILE COVERS 1907 - 21 Jul 2003 VOL 139 ISS 4
FILE LAST UPDATED: 20 Jul 2003 (20030720/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que 132

L1	1299	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	170
L2	20	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L1 AND "WATER"
L3	17	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L2 AND " WATER-170"
L4	4	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L3 AND H2O/MF
L5	4	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L4 AND NC=1
L6	2	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L5 NOT T/ELS
L7	1	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	15587-57-2 $H_2^{17}O$
L8	169	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	(L6 OR L7)
L25	56	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L8 AND (NMR OR MAGNETIC)/OBI
L32	9	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L25 AND TISSUE

nc = # components

T = Tritium

els = element symbol

obi = all search fields except for abstract

=> d que 133

L1	1299	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	170
L2	20	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L1 AND "WATER"
L3	17	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L2 AND " WATER-170"
L4	4	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L3 AND H2O/MF
L5	4	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L4 AND NC=1
L6	2	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L5 NOT T/ELS
L7	1	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	15587-57-2
L8	169	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	(L6 OR L7)
L25	56	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L8 AND (NMR OR MAGNETIC)/OBI
L26	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L25 AND COMPOSITION
L27	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L25 AND (BOLUS OR LIPOSOM?)
L28	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L25 AND DIAGNOS?
L29	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L25 AND ORGAN
L30	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L25 AND DISEASE
L31	2	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	L25 AND (AMINO ACID)
L33	8	SEA	FILE=HCAPLUS	ABB=ON	PLU=ON	(L26 OR L27 OR L28 OR L29 OR L30 OR L31)

8 cites

=> d que 174

L1 1299 SEA FILE=REGISTRY ABB=ON PLU=ON 170
 L2 20 SEA FILE=REGISTRY ABB=ON PLU=ON L1 AND "WATER"
 L3 17 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND "WATER-170"
 L4 4 SEA FILE=REGISTRY ABB=ON PLU=ON L3 AND H2O/MF
 L5 4 SEA FILE=REGISTRY ABB=ON PLU=ON L4 AND NC=1
 L6 2 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT T/ELS
 L7 1 SEA FILE=REGISTRY ABB=ON PLU=ON 15587-57-2
 L8 169 SEA FILE=HCAPLUS ABB=ON PLU=ON (L6 OR L7)
 L11 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L8 AND (PHARMA? OR DRUG)
 L15 44081 SEA FILE=HCAPLUS ABB=ON PLU=ON DIAGNOSIS+PFT/CT
 L16 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 AND L8
 L17 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L8(L) (DGN)/RL
 L19 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L8 AND SOLVENT
 L20 19 SEA FILE=HCAPLUS ABB=ON PLU=ON L8 AND SOLUTION
 L21 18 SEA FILE=HCAPLUS ABB=ON PLU=ON L20 NOT L19
 L22 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L21 AND HYDRATION NUMBER/OBI
 L23 4954 SEA FILE=HCAPLUS ABB=ON PLU=ON IMAGING AGENTS+PFT,NT/CT
 L24 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L23 AND L8
 L74 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 OR (L16 OR L17) OR L22 OR
 L24 6 cites

PFT = old, now $\frac{1}{2}$ "used
for" terms

CT = controlled
terminology

DGN = diagnosis
RL = role

NT = narrower
term

=> s 132-33 or 174

L103 13 (L32 OR L33) OR L74

=> file wpix

FILE 'WPIX' ENTERED AT 17:27:55 ON 21 JUL 2003
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FILE LAST UPDATED: 19 JUL 2003 <20030719/UP>
MOST RECENT DERWENT UPDATE: 200346 <200346/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> NEW WEEKLY SDI FREQUENCY AVAILABLE --> see NEWS <<<

>>> SLART (Simultaneous Left and Right Truncation) is now
available in the /ABEX field. An additional search field
/BIX is also provided which comprises both /BI and /ABEX <<<

>>> PATENT IMAGES AVAILABLE FOR PRINT AND DISPLAY <<<

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>>> FOR INFORMATION ON ALL DERWENT WORLD PATENTS INDEX USER
GUIDES, PLEASE VISIT:
http://www.derwent.com/userguides/dwpi_guide.html <<<

=> d que 180

L76 75 SEA FILE=WPIX ABB=ON PLU=ON 170 OR OXYGEN-17
 L77 1190844 SEA FILE=WPIX ABB=ON PLU=ON H2O OR WATER
 L78 26 SEA FILE=WPIX ABB=ON PLU=ON L76 AND L77

L80 5 SEA FILE=WPIX ABB=ON PLU=ON L78 AND (DRUG OR PHARMACEUT? OR THERAP?) *5 cites*

=> d que 182

L76 75 SEA FILE=WPIX ABB=ON PLU=ON 170 OR OXYGEN-17
 L77 1190844 SEA FILE=WPIX ABB=ON PLU=ON H2O OR WATER
 L78 26 SEA FILE=WPIX ABB=ON PLU=ON L76 AND L77
 L80 5 SEA FILE=WPIX ABB=ON PLU=ON L78 AND (DRUG OR PHARMACEUT? OR THERAP?)
 L81 21 SEA FILE=WPIX ABB=ON PLU=ON L78 NOT L80
 L82 6 SEA FILE=WPIX ABB=ON PLU=ON L81 AND (YEAST OR TOMOGRAPHY OR PARENTERAL OR BURNS OR LIPOSOME OR MICROCLUSTER) *6 cites*

=> s 180 or 182

L104 11 L80 OR L82 *11 cites for per ment*

=> dup rem 1103 1104

FILE 'HCAPLUS' ENTERED AT 17:28:37 ON 21 JUL 2003
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FILE 'WPIX' ENTERED AT 17:28:37 ON 21 JUL 2003
 COPYRIGHT (C) 2003 THOMSON DERWENT
 PROCESSING COMPLETED FOR L103
 PROCESSING COMPLETED FOR L104

L105 23 DUP REM L103 L104 (1 DUPLICATE REMOVED) *23 cites total*
 ANSWERS '1-13' FROM FILE HCAPLUS
 ANSWERS '14-23' FROM FILE WPIX

=> d ibib abs ind 1-13 *ind = indexing*

L105 ANSWER 1 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STNDUPLICATE 1 *applicants*
 ACCESSION NUMBER: 2000:98382 HCAPLUS
 DOCUMENT NUMBER: 132:134185
 TITLE: **Drugs for therapeutic use enabling nuclear magnetic resonance diagnosis by scalar bond**
 INVENTOR(S): Washino, Komei; Shimmura, Toshiyuki; Nakatani, Akira; Fujimoto, Chieko; Tanaka, Akihiro; Seri, Shigemi; Iwai, Kumiko
 PATENT ASSIGNEE(S): Nihon Medi-Physics Co., Ltd., Japan
 SOURCE: PCT Int. Appl., 15 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000006207	A1	20000210	WO 1999-JP3970	19990723
W: AU, BR, CA, CN, KR, NO, NZ, RU, US, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2000044491	A2	20000215	JP 1998-213050	19980728
CA 2338702	AA	20000210	CA 1999-2338702	19990723

AU 9948005 A1 20000221 AU 1999-48005 19990723
 AU 758913 B2 20030403
 EP 1101498 A1 20010523 EP 1999-931523 19990723
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, FI

NO 2001000423 A 20010124 NO 2001-423 20010124
 PRIORITY APPLN. INFO.: JP 1998-213050 A 19980728
 WO 1999-JP3970 W 19990723

AB **Drugs** for therapeutic use characterized by contg. a compd. which carries in its structure at least one member selected from among -17OH, -14NH and -33SH, wherein the above 17O, 14N or 33S exerts a relaxation effect on the proton bonded thereto and the relaxation effect is transported through the exchange of a proton in a vital component of a target **organ** or **tissue** by the above-mentioned proton, thus enabling detection by NMR. The effective circulation or distribution of such a physiol. acceptable therapeutic **drug** in the target **organ** or **tissue** in vivo where it is needed can be externally detected by the NMR method before the administration of a remedy to each patient or simultaneously therewith.

IC ICM A61K049-00

CC 8-9 (Radiation Biochemistry)

Section cross-reference(s): 63

ST radiopharmaceutical **diagnosis** NMR MRI scalar bond;
 infusion **liposome** radiopharmaceutical **diagnosis**
 NMR MRI

IT **Diagnosis**

(agents; **drugs** for therapeutic use enabling NMR
diagnosis by scalar bond)

IT Animal tissue

Drug delivery systems

Imaging agents

NMR (nuclear magnetic resonance)

Organ, animal

Positron-emission tomography

(**drugs** for therapeutic use enabling NMR

diagnosis by scalar bond)

IT Amino acids, biological studies

RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

(**drugs** for therapeutic use enabling NMR

diagnosis by scalar bond)

IT Drug delivery systems

(infusions; **drugs** for therapeutic use enabling NMR

diagnosis by scalar bond)

IT Drug delivery systems

(**liposomes**; **drugs** for therapeutic use enabling

NMR **diagnosis** by scalar bond)

IT 257283-87-7P, D-Glucose-3-170 257283-88-8P, D-Glucose-1-170

RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(**drugs** for therapeutic use enabling NMR

diagnosis by scalar bond)

IT 50-21-5, Lactic acid, biological studies 50-99-7, Glucose, biological studies 4033-40-3, N-Acetyl asparagine 7727-37-9, Nitrogen, biological studies 12586-59-3, Proton 13774-92-0, Imidogen 13968-48-4, biological studies 14257-58-0, S-33, biological studies 15587-57-2, Hydroxyl-170 31713-49-2, Mercapto-33S

RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)

I included the indexing terms because they cover all of the topics in the full paper. The abstract sometimes misses topics

*Indexing
terms*

(drugs for therapeutic use enabling NMR
diagnosis by scalar bond)
IT 19646-38-9, p-Toluene sulfonyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(drugs for therapeutic use enabling NMR
diagnosis by scalar bond)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L105 ANSWER 2 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:266880 HCAPLUS
DOCUMENT NUMBER: 138:276318
TITLE: NMR imaging diagnostic agents
containing 170-water
INVENTOR(S): Otsuka, Akihiro; Nakaya, Akira; Iwai, Kumiko
PATENT ASSIGNEE(S): Nihon Medipysics Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003102698	A2	20030408	JP 2001-301681	20010928
WO 2003028769	A1	20030410	WO 2002-JP9872	20020925

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT,
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG,
US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 2001-301681 A 20010928
AB The agents, useful for anal. of tissue perfusion (e.g., blood
flow), are biol. acceptable aq. solns. contg. mols. having H atom directly
bonded to quadrupole nucleus and showing (a) T2 relaxation .gtoreq.0.1
s-lat.%-1 and/or (b) inhibition of change in biol. information after
bolus dose. A soln. contg. 0.9% NaCl in H2O contg. 5 at.% H217O
showed 0.17-1.1 s-lat.%-1 T2 relaxation at pH 5.0-8.0.
IC ICM A61B005-055
ICS A61K049-00; G01R033-28
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 9
ST NMR imaging diagnostic agent T2 relaxation; blood flow
analysis NMR diagnostic agent; sodium chloride
NMR imaging diagnostic agent
IT Imaging agents
(NMR contrast; NMR imaging diagnostic
agents contg. 170-water and biol. ions)
IT Diagnosis
(agents; NMR imaging diagnostic agents contg.
170-water and biol. ions)
IT Circulation
(anal.; NMR imaging diagnostic agents contg.
170-water and biol. ions)

IT 7440-09-7, Potassium, biological studies 7440-23-5, Sodium, biological studies 7440-70-2, Calcium, biological studies 7647-14-5, Sodium chloride, biological studies 13768-40-6, Water-170
 RL: DGN (Diagnostic use); BIOL (Biological study); USES (Uses)
 (NMR imaging diagnostic agents contg. 170-water and
 biol. ions)

L105 ANSWER 3 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:10813 HCAPLUS

DOCUMENT NUMBER: 136:66628

TITLE: Imaging methods for visualizing implanted living cells

INVENTOR(S): Moseley, Michael E.; Kucharczyk, John

PATENT ASSIGNEE(S): The Regents of the University of Minnesota, USA; The Board of Trustees of the Leland Stanford Jr. University

SOURCE: PCT Int. Appl., 35 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002001242	A2	20020103	WO 2001-US17403	20010530
WO 2002001242	A3	20020613		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR

PRIORITY APPLN. INFO.: US 2000-606137 A 20000628

AB Cell transplantation is becoming an increasingly important method of therapy for patients. There has been no uniform methodol. or instrumentality for relatively non-invasive observation of the progression or success of the cell implantation. A method is provided herein for indicating viability of transplanted cells with a medical device that supports at least one sensing function comprising: non-destructively observing a region of a patient to where cells have been transplanted; guiding the medical device to said region of a patient using the non-destructive observation; positioning said medical device within said region of a patient using the non-destructive observation to assist in the positioning; sensing a property within said region of a patient that is indicative of cell viability or inviability; and using data from sensing said property within said region to indicate cell viability from a transplant with the region. Magnetic Resonance Imaging is a particularly useful format for non-destructive observation of the region. As an example, cell viability may indicated by a property resulting from an event selected from the group consisting of the cell activity, cell inactivity, cell growth, cell death, specific cell function, specific cell dysfunction, volumetric expansion of cell population, and volumetric decrease of cell population, while the property may be detd. with monitoring by at least one technique selected from the group consisting of proton spectroscopy, monitoring of C-13 labeled glucose, monitoring by P-31 MR spectroscopy, monitoring of local F-19 labeled metabolites, monitoring of Na-23 levels, and monitoring of 17O2 gas conversion to H217O water.

IC ICM G01R033-46
 ICS A61B005-00; G01R033-563; A61B005-04; A61B005-055
 CC 9-16 (Biochemical Methods)
 Section cross-reference(s): 1, 8, 63
 ST imaging visualizing implanted living cell
 IT Optical imaging devices
 (NMR, RF coil; imaging methods for visualizing implanted
 living cells)
 IT Imaging
 (NMR; imaging methods for visualizing implanted living cells)
 IT Coloring materials
 (Optically-active; imaging methods for visualizing implanted living
 cells)
 IT Stress, animal
 (Oxygenation; imaging methods for visualizing implanted living cells)
 IT Metabolism, animal
 (Phosphorous high-energy metabolites; imaging methods for visualizing
 implanted living cells)
 IT Spectroscopy
 (Proton; imaging methods for visualizing implanted living cells)
 IT Electric properties
 (biol.; imaging methods for visualizing implanted living cells)
 IT **Imaging agents**
 (contrast; imaging methods for visualizing implanted living cells)
 IT Information systems
 (data; imaging methods for visualizing implanted living cells)
 IT Animal cell
 Animal **tissue**
 Cell death
 Cell proliferation
 Circulation
 Concentration (condition)
 Density
 Diffusion
 Electric impedance
 Fluorescence
 Imaging
 Luminescence, bioluminescence
 Materials
 Medical goods
 Oxidation
 Temperature
 Transplant and Transplantation
 Volume
 (imaging methods for visualizing implanted living cells)
 IT Hemoglobins
 Hemoglobins, oxyhemoglobins
 RL: ANT (Analyte); ANST (Analytical study)
 (imaging methods for visualizing implanted living cells)
 IT Energy-rich phosphates
 RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical
 study); BIOL (Biological study)
 (imaging methods for visualizing implanted living cells)
 IT Brain, **disease**
 (ischemia, focal; imaging methods for visualizing implanted living
 cells)
 IT NMR spectroscopy
 (phosphorus-31; imaging methods for visualizing implanted living cells)
 IT Spin-lattice relaxation
 Spin-spin relaxation

(shortening agents; imaging methods for visualizing implanted living cells)

IT 56-12-2, .gamma.-Aminobutyric acid, analysis 57-00-1, Creatine
62-49-7, Choline 107-73-3, Phosphocholine 997-55-7

RL: ANT (Analyte); ANST (Analytical study)

(imaging methods for visualizing implanted living cells)

IT 50-21-5, analysis 50-99-7, Glucose, analysis 7440-23-5, Sodium-23,
analysis 7732-18-5, Water, analysis 7782-41-4D, Fluorine-19,
metabolites labeled with, analysis 7782-44-7, Oxygen, analysis
13768-40-6, Water-17O 13968-48-4, Oxygen 17, analysis

19030-38-7, Glucose, labeled with carbon 13, analysis

RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)

(imaging methods for visualizing implanted living cells)

IT 7440-63-3, Xenon, biological studies

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES
(Uses)

(imaging methods for visualizing implanted living cells)

L105 ANSWER 4 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:690948 HCAPLUS

DOCUMENT NUMBER: 128:45418

TITLE: Strong and weak binding of water to proteins studied
by NMR triple-quantum filtered relaxation
spectroscopy of 17O-water

AUTHOR(S): Torres, Allan M.; Grieve, Stuart M.; Chapman, Bogdan
E.; Kuchel, Philip W.

CORPORATE SOURCE: Department of Biochemistry, the University of Sydney,
Sydney, N.S.W., Australia

SOURCE: Biophysical Chemistry (1997), 67(1-3), 187-198
CODEN: BICIAZ; ISSN: 0301-4622

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The triple-quantum filtered (TQF) spin-echo signal of 17O-water, in the
presence of proteins, was analyzed to yield ests. of the no. of weakly,
and strongly bound water mols. The anal. used a constrained direct
iterative regression procedure with a three-state model of fast-exchange.
Thus, the population size of free, weakly, and strongly bound water were
detd. simultaneously. The two fractions of the bound water were estd. by
using correlation time(s) estd. in other studies. Bovine serum albumin
(BSA), basic pancreatic trypsin inhibitor (BPTI), lysozyme and oxyHb were
studied. Of the four proteins, BSA contained the largest no. of strongly
and weakly bound water mols., there being .apprx.30 of the former and
.apprx.3000 of the latter under conditions of high protein concn. The
correlation time of the proteins increases with their concn. in soln., and
when this was taken into account for BSA the estd. no. of strongly bound
water mols. did not change significantly. This NMR technique, and data
anal., will probably also be useful in studies of water binding and
mobility in various systems including hydrogels, protein networks,
membranes, cells and tissues.

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 6, 7, 61

ST water binding protein TQF NMR spectrometry; triple quantum
filtered relaxation NMR spectroscopy

IT Albumins, biological studies

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
(Biological study)

(serum; strong and weak binding of water to proteins studied by
NMR triple-quantum filtered relaxation spectroscopy of

170-water)
IT Hydration, chemical
(strong and weak binding of water to proteins studied by NMR
triple-quantum filtered relaxation spectroscopy of 170-water)
IT Hemoglobins, oxyhemoglobins
Proteins, general, biological studies
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
(Biological study)
(strong and weak binding of water to proteins studied by NMR
triple-quantum filtered relaxation spectroscopy of 170-water)
IT NMR spectroscopy
(triple-quantum filtered relaxation; strong and weak binding of water
to proteins studied by NMR triple-quantum filtered relaxation
spectroscopy of 170-water)
IT 7732-18-5, Water, biological studies 9001-63-2, Lysozyme 9087-70-1,
BPTI 13768-40-6, Water-170
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
(Biological study)
(strong and weak binding of water to proteins studied by NMR
triple-quantum filtered relaxation spectroscopy of 170-water)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L105 ANSWER 5 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:392466 HCAPLUS

DOCUMENT NUMBER: 125:142040

TITLE: Hydration of amines, diamines, polyamines and amides
studied by NMR

AUTHOR(S): Okouchi, Shoichi; Moto, Tetsuhi; Ishihara, Yoshimasa;
Numajiri, Haruhiko; Uedaira, Hisashi

CORPORATE SOURCE: Kameyama, T.; Nakamura, T.; Ueda, T.; Hirasawa,
Dep. Mater. Chem., Hosei Univ., Koganei, 184, Japan
SOURCE: Journal of the Chemical Society, Faraday Transactions
(1996), 92(11), 1853-1857
CODEN: JCFTEV; ISSN: 0956-5000

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The spin-lattice relaxation times, T_1 , of natural abundance H21170 have been measured for aq. solns. of nine amines, five diamines, two polyamines and five amides, as a function of the concn. at 25.degree.C. The water-accessible surface areas of the solute mols. were calcd.. The coordination no., nh, and the rotational correlation times, τ_{ch} , of water mols. around the solute mols. were estd. and compared with that of pure water τ_{c0} . The value of $\tau_{ch}/\tau_{c0} = 2.02$ for tert-butylamine is the largest and that of $\tau_{ch}/\tau_{c0} = 0.97$ for urea the smallest obtained. The value of nh ($\tau_{ch}/\tau_{c0} - 1$) was defined as the dynamic hydration no. (DHN). The partial molar vols. and the partial molar heat capacities for these homologues at infinite diln. are linearly dependent on their DHN.

CC 22-13 (Physical Organic Chemistry)

ST amine NMR hydration; diamine NMR hydration; polyamine NMR hydration; amide NMR hydration

IT Hydration, chemical

Hydration number

(dynamic; hydration of amines, diamines, polyamines and amides examd. by NMR)

IT Homologous series

(hydration of amines, diamines, polyamines and amides examd. by NMR)

IT Amines, properties

RL: PRP (Properties)

- (hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT Amides, reactions
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT Molecules
(surface area; hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT Amines, properties
RL: PRP (Properties)
(di-, hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT Molar volume and Molecular volume
(partial, hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT Heat capacity
(partial molar, hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT Amines, properties
RL: PRP (Properties)
(poly-, hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT Magnetic relaxation
(spin-lattice, 170; hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT 13768-40-6, Water-170
RL: NUU (Other use, unclassified); PRP (Properties); USES (Uses)
(hydration of amines, diamines, polyamines and amides examd. by NMR)
- IT 57-13-6, Urea, properties 60-35-5, Acetamide, properties 71-44-3
74-89-5, Methylamine, properties 75-04-7, Ethylamine, properties
75-31-0, Isopropylamine, properties 75-64-9, tert-Butylamine, properties
78-81-9, Isobutylamine 79-05-0, Propionamide 107-10-8, Propylamine,
properties 107-15-3, 1,2-Ethanediamine, properties 109-73-9,
Butylamine, properties 109-76-2, 1,3-Propanediamine 110-58-7,
1-Pentanamine 110-60-1, 1,4-Butanediamine 124-09-4, 1,6-Hexanediamine,
properties 124-20-9 462-94-2, 1,5-Pentanediamine 626-97-1,
Pentanamide 628-02-4, Hexanamide 13952-84-6, Sec-Butylamine
RL: PRP (Properties)
(hydration of amines, diamines, polyamines and amides examd. by NMR)

L105 ANSWER 6 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:811831 HCAPLUS

DOCUMENT NUMBER: 123:250191

TITLE: Detection of 170 by proton T1.rho. dispersion imaging

AUTHOR(S): Reddy, Ravinder; Stolpen, Alan H.; Leigh, J. S.

CORPORATE SOURCE: Dep. Radiology MMRRCC, Stellar-Chance Lab., School
Medicine, University Pennsylvania, Philadelphia, PA,
19104-6100, USA

SOURCE: Journal of Magnetic Resonance, Series B (1995),
108(3), 276-9

CODEN: JMRBE5; ISSN: 1064-1866

PUBLISHER: Academic

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effect of 170-enriched water on proton T1 relaxation enhancement in
aq. phantoms was examd. at high magnetic field strength. H2170 produced
marked enhancement of proton T1 relaxation in aq. phantoms. The method
has potential applications in functional magnetic resonance imaging,
particularly in the measurement of tissue perfusion and
oxidative metab.

CC 8-9 (Radiation Biochemistry)

ST oxygen 17 NMR imaging phantom
 IT Imaging
 (NMR, 170 NMR imaging of aq. phantom)
 IT Magnetic relaxation
 (spin-lattice, 170 NMR imaging of aq. phantom)
 IT 13768-40-6, Water-170
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (170 NMR imaging of aq. phantom)

L105 ANSWER 7 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:26749 HCAPLUS

DOCUMENT NUMBER: 120:26749

TITLE: Effects of oxygen-17-labeled water on the backbone
 amide proton relaxation rates of the
 [U-15N]FKBP/ascomycin complex

AUTHOR(S): Yu, Liping; Olejniczak, Edward T.; Fesik, Stephen W.
 CORPORATE SOURCE: Pharm. Discov. Div., Abbott Lab., Abbott park, IL,
 60064, USA

SOURCE: Journal of Magnetic Resonance, Series B (1993),
 102(2), 218-21
 CODEN: JMRBES; ISSN: 1064-1866

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The method of C. H. Lin et al. (1991), which depends on the change in the
 1H NMR relaxation rates of a biomacromol. in the presence of 170-labeled
 water and which was tested on a DNA/drug adduct, was evaluated
 on the well-characterized FK506-binding protein (FKBP)/ascomycin complex
 by comparing the T1 and T2 relaxation times of the backbone amide protons
 of FKBP in the presence of 160-labeled water vs. 170-labeled water.
 Results from the FKBP/ascomycin complex are contradictory to the earlier
 observations of Lin et al. and suggest that their results are probably not
 due simply to water mol. tightly bound to the DNA/drug adduct.

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 77

ST biopolymer bound water detection NMR spectrometry; proton magnetic
 relaxation protein water; FKBP ascomycin complex water magnetic relaxation

IT Water of hydration
 (detn. of location of, on biomacromols. by NMR spectrometry)

IT Biopolymers
 Proteins, biological studies
 RL: ANST (Analytical study)
 (water bound to, detn. of location of, by NMR spectrometry)

IT Proteins, specific or class
 RL: ANST (Analytical study)
 (FKBP (FK 506-binding protein), complexes with ascomycin, water labeled
 with oxygen-17 effect on backbone amide proton relaxation rates of)

IT Macromolecular compounds
 RL: ANST (Analytical study)
 (biol., water bound to, detn. of location of, by NMR spectrometry)

IT Magnetic relaxation
 (spin-lattice, of protons of backbone amides in FK 506-binding
 protein-ascomycin complex)

IT Magnetic relaxation
 (spin-spin, of protons of backbone amides in FK 506-binding
 protein-ascomycin complex)

IT 13768-40-6, Water-170
 RL: ANST (Analytical study)
 (proton relaxation rates of backbone amides of FK 506-binding
 protein-ascomycin complex response to)

IT 104987-12-4D, Ascomycin, complexes with FK 506-binding protein

RL: ANST (Analytical study)
 (water labeled with oxygen-17 effect on backbone amide proton
 relaxation rates of)

L105 ANSWER 8 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1993:72207 HCAPLUS

DOCUMENT NUMBER: 118:72207

TITLE: NMR relaxation in binary aqueous mixtures of
 acetone and tetrahydrofuran

AUTHOR(S): Ludwig, R.; Zeidler, M. D.

CORPORATE SOURCE: Inst. Phys. Chem., RWTH, Aachen, D-5100, Germany

SOURCE: Journal of Molecular Liquids (1992), 54(4), 181-91
 CODEN: JMLIDT; ISSN: 0167-7322

DOCUMENT TYPE: Journal

LANGUAGE: English

- AB NMR proton relaxation rates of normal and 17O-enriched H2O and deuterium
 relaxation rates of D2O were measured in mixts. with acetone and THF at
 different **compns.** The 17O-induced proton relaxation rate was
 extd. and from this the rotational correlation time of H2O was detd.
 Using these correlation times the **compn.** dependence of the
 deuterium quadrupole coupling const. of H2O was derived. A strong
 variation was found for the system acetone-H2O, whereas little variation
 was obsd. for THF-H2O.
- CC 77-7 (Magnetic Phenomena)
- ST NMR relaxation acetone THF aq mixt; quadrupole coupling water
 deuterium; proton relaxation oxygen 17 water; rotation correlation water
 acetone THF mixt
- IT Quadrupole coupling
 (deuterium, of water in acetone-tetrahydrofuran aq. mixts.)
- IT Molecular rotation
 (of water in acetone-tetrahydrofuran aq. mixts., correlation time of)
- IT **Magnetic** relaxation
 (spin-lattice, in acetone-tetrahydrofuran aq. mixts.)
- IT 67-64-1, Acetone, properties
 RL: PRP (Properties)
 (nuclear spin-lattice relaxation in aq. mixts. of THF and)
- IT 109-99-9, Tetrahydrofuran, properties
 RL: PRP (Properties)
 (nuclear spin-lattice relaxation in aq. mixts. of acetone and)
- IT 7732-18-5, Water, properties
 RL: PRP (Properties)
 (rotational correlation time of, in acetone-tetrahydrofuran aq. mixts.)
- IT 7789-20-0, Water-d2
 RL: PRP (Properties)
 (spin-lattice relaxation of deuterium in mixts. of acetone and THF and)
- IT **13768-40-6**, Water-17O
 RL: PRP (Properties)
 (spin-lattice relaxation of proton in mixts. of acetone and THF and)

L105 ANSWER 9 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1992:210372 HCAPLUS

DOCUMENT NUMBER: 116:210372

TITLE: The stability of proton T2 effects of oxygen-17-water
 in experimental cerebral ischemia

AUTHOR(S): Hopkins, A. L.; Lust, W. D.; Haacke, E. M.;

Wielopolski, P.; Barr, R. G.; Bratton, C. B.

CORPORATE SOURCE: Dep. Anat., Case West. Reserve Univ., Cleveland, OH,
 44106, USA

SOURCE: Magnetic Resonance in Medicine (1991), 22(1), 167-74
 CODEN: MRMEEN; ISSN: 0740-3194

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The gerbil model of unilateral cerebral ischemia has been used to test the temporal and spatial stability of the magnetic resonance imaging (MRI) T2 effects of [17O]water (H217O). Following unilateral carotid ligation, symptomatic animals were given a single large i.p. injection of H217O and the distribution and stability of the brain T2 effects were followed with a spin-echo sequence. In contrast to the ischemic area, the perfused **tissue** shows a marked and prolonged loss in intensity with little evidence of diffusion of the T2 effect of 17O into the ischemic **tissue**.

CC 8-9 (Radiation Biochemistry)
 Section cross-reference(s): 14

ST brain ischemia NMR imaging; oxygen 17 water imaging brain ischemia

IT Imaging
 (NMR, of brain ischemia, with oxygen-17-water)

IT Brain, **disease**
 (ischemia, NMR imaging of, with oxygen-17-water)

IT **Magnetic** relaxation
 (spin-spin, of brain ischemia, using oxygen-17-water, stability of, imaging in relation to)

IT **13768-40-6**, Water-17O
 RL: BIOL (Biological study)
 (NMR imaging with, of brain ischemia)

L105 ANSWER 10 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:406771 HCAPLUS

DOCUMENT NUMBER: 113:6771

TITLE: Natural-abundance oxygen-17 **magnetic** relaxation in aqueous **solutions** of apolar **amino acids** and glycine peptides

AUTHOR(S): Ishimura, Miyuki; Uedaira, Hisashi
 CORPORATE SOURCE: Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan
 SOURCE: Bulletin of the Chemical Society of Japan (1990), 63(1), 1-5
 CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The spin-lattice relaxation times, T1, of H217O have been measured for the aq. **solns.** of 11 apolar **amino acids** and 5 glycine peptides, as a function of the concn. at 25.degree.. The coordination nos., nh, and the rotational correlation times, .tau.ch, of water mols. around the **amino acids** and peptides were estd. and compared with that of pure water, .tau.c0. The value of .tau.ch/.tau.c0 = 1.87 for norleucine is the largest, while those of .tau.c/.tau.c0 for glycine peptides are almost the same, 1.2. The value of nh(.tau.ch/.tau.c0-1) was defined as the dynamic hydration no. (DHN). The DHN showed a good correlation with several physicochem. properties, such as the mol. wts., partial molar volumes, adiabatic compressibilities, heat capacities, B-coeffs. of the activity coeff., and limiting diffusion coeffs. of **amino acids** and glycine peptides in aq. **solns.**

CC 34-2 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 22

ST dynamic **hydration number** **amino acid**
 ; glycine oligomer dynamic **hydration number**; oxygen 17 NMR relaxation **amino acid**; thermodyn structure property relationship

IT **Hydration number**

- (dynamic, of amino acids and glycine oligomers, by oxygen-17 magnetic relaxation of aq. solns.)
- IT Amino acids, properties
RL: PRP (Properties)
(oxygen-17 magnetic relaxation of soln. of, thermodyn. properties in relation to)
- IT Magnetic relaxation
(spin-lattice, of oxygen-17 in aq. solns. of amino acids and glycine oligomers, thermodyn. properties in relation to)
- IT Molecular structure-property relationship
(thermodyn., of amino acids and glycine oligomers, by oxygen-17 magnetic relaxation of aq. solns.)
- IT 56-12-2, .gamma.-Aminobutyric acid, properties 56-40-6, Glycine, properties 56-41-7, L-Alanine, properties 61-90-5, L-Leucine, properties 72-18-4, Valine, properties 73-32-5, Isoleucine, properties 107-95-9, .beta.-Alanine 327-57-1, Norleucine 541-48-0, .beta.-Aminobutyric acid 556-33-2, Triglycine 556-50-3, Diglycine 637-84-3, Tetraglycine 2835-81-6, .alpha.-Aminobutyric acid 3887-13-6, Hexaglycine 6600-40-4, Norvaline 7093-67-6, Pentaglycine
RL: PRP (Properties)
(oxygen-17 magnetic relaxation of soln. of, thermodyn. properties in relation to)
- IT 13768-40-6, Water-170
RL: PROC (Process)
(spin-lattice relaxation of, in the presence of amino acids and glycine oligomers, thermodyn. properties in relation to)

L105 ANSWER 11 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1989:36214 HCAPLUS

DOCUMENT NUMBER: 110:36214

TITLE: Oxygen-17 contrast agents. Fast imaging techniques

AUTHOR(S): Hopkins, Amos L.; Haacke, E. Mark; Barr, Richard G.; Tkach, Jean

CORPORATE SOURCE: Dep. Anat., Case Western Reserve Univ., Cleveland, OH, USA

SOURCE: Investigative Radiology (1988), 23(Suppl. 1), S240-S242

CODEN: INVRAV; ISSN: 0020-9996

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Under physiol. conditions, the stable isotope ^{17}O , in the form of H_2^{17}O , lowers the proton T_2 of blood, cerebrospinal fluid, tissues, and whole organisms. With magnetic resonance imaging the resulting changes in intensity can be detected using spin-echo pulse sequences, but much greater sensitivity is achieved in a fraction of the time with a steady-state free precession sequence such as FISP (fast imaging with steady precision). With this sequence, it is possible to detect levels of $\geq 0.4\%$ ^{17}O water in ≤ 53 s.

CC 8-9 (Radiation Biochemistry)

ST magnetic resonance imaging oxygen 17

IT Cerebrospinal fluid

Kidney

(magnetic resonance imaging of, oxygen-17 contrast agents for)

IT Blood

Blood plasma

(magnetic spin-spin relaxation of, oxygen-17 as contrast agent for, imaging in relation to)

- IT Albumins, properties
RL: PRP (Properties)
(magnetic spin-spin relaxation of, oxygen-17 as contrast agent for, imaging in relation to)
- IT Tomography
(NMR, of organs and tissues, oxygen-17 contrast agents for)
- IT Magnetic relaxation
(spin-spin, imaging by, of organs and tissues, oxygen-17 contrast agents for)
- IT 13768-40-6, Water-17O 13968-48-4, Oxygen-17, biological studies
RL: BIOL (Biological study)
(contrast agent, for NMR imaging of organs and tissues)

L105 ANSWER 12 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1987:403416 HCAPLUS

DOCUMENT NUMBER: 107:3416

TITLE: Oxygen-17 compounds as potential NMR T2 contrast agents: enrichment effects of 17O-water on protein solutions and living tissues

AUTHOR(S): Hopkins, A. L.; Barr, R. G.

CORPORATE SOURCE: Dep. Dev. Genet. Anat., Case Western Reserve Univ., Cleveland, OH, 44106, USA

SOURCE: Magnetic Resonance in Medicine (1987), 4(4), 399-403
CODEN: MRMEEN; ISSN: 0740-3194

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The isotopic enrichment of solns., living tissues, and organisms with 17O in the form of H217O shortens their proton NMR transverse relaxation times (T2) and produces changes in NMR image intensity. The transverse relaxation rate (1/T2) was linearly dependent on the H217O concn. in biol. solns. up to 5% enrichment. The longitudinal relaxation time (T1) is not affected by enrichment. Equal concns. of H217O do not produce the same magnitude of T2 change in all physiol. environments. The reasons for these differences are discussed. The results suggest that certain 17O compds. should be explored as contrast agents in magnetic resonance imaging.

CC 8-9 (Radiation Biochemistry)

ST NMR imaging tissue oxygen 17

IT Kidney

(NMR imaging of, oxygen-17 compds. as contrast agents for)

IT Blood

Blood plasma

Cerebrospinal fluid

(magnetic spin-spin relaxation time of oxygen-17 in, NMR imaging in relation to)

IT Albumins, properties

RL: PRP (Properties)

(magnetic spin-spin relaxation times in solns. of, oxygen-17 effect on, NMR imaging in relation to)

IT Tomography

(NMR, of animal tissues, oxygen-17 compds. as contrast agents for)

IT Magnetic relaxation

(spin-spin, imaging by, of animal tissues, oxygen-17 compds. as contrast agents for)

IT 13768-40-6 13968-48-4, Oxygen-17, properties

RL: BIOL (Biological study)

(magnetic spin-spin relaxation time in protein solns. and

tissues response to, NMR imaging in relation to)

L105 ANSWER 13 OF 23 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1987:511880 HCAPLUS
 DOCUMENT NUMBER: 107:111880
 TITLE: Proton transverse relaxation rate of oxygen-17-enriched water
 AUTHOR(S): Yeung, Hong N.; Lent, Arnold H.
 CORPORATE SOURCE: Technicare Corp., Solon, OH, 44139, USA
 SOURCE: Magnetic Resonance in Medicine (1987), 5(1), 87-92
 CODEN: MRMEEN; ISSN: 0740-3194
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Proton transverse relaxation rates of 17O-enriched water at pH in the neutral range were detd. with isotopic **compns.** of 17O varying from natural abundance to 5%. S. Meiboom's (1961) account of the proton 1/T2 caused by the scalar interaction between the proton and 17O is generalized to accommodate new data. The generalized formulation covers 17O enrichment above the limit to which Meiboom and his coworker constrained all their work.
 CC 8-9 (Radiation Biochemistry)
 ST **magnetic** relaxation oxygen 17 water; imaging NMR
 IT **tissue oxygen 17**
 IT Cerebrospinal fluid
 (NMR imaging of, oxygen-17-enriched water spin-spin
magnetic relaxation in relation to)
 IT Tomography
 (NMR, of animal **tissues**, oxygen-17-enriched water
 spin-spin **magnetic** relaxation in relation to)
 IT **Magnetic** relaxation
 (spin-spin, of oxygen-17-enriched water, **tissue** imaging in
 relation to)
 IT **13768-40-6, Water-17O**
 RL: BIOL (Biological study)
 (**magnetic** relaxation of, spin-spin, **tissue** imaging
 in relation to)

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L105 ANSWER 14 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
 ACCESSION NUMBER: 2002-590607 [63] WPIX
 DOC. NO. NON-CPI: N2002-468674
 DOC. NO. CPI: C2002-167066
 TITLE: Identifying a differentially expressed protein in two different samples, useful for rapid identification of marker or target proteins that can be applied in the study of e.g. **drug** toxicity, by performing inverse labeling of proteins.
 DERWENT CLASS: B04 J04 K08 S03
 INVENTOR(S): FU, E W; MA, Z; QUINN, D F; WANG, Y K
 PATENT ASSIGNEE(S): (FUEW-I) FU E W; (MAZZ-I) MA Z; (QUIN-I) QUINN D F; (WANG-I) WANG Y K; (NOVS) NOVARTIS AG; (NOVS) NOVARTIS-ERFINDUNGEN VERW GES MBH
 COUNTRY COUNT: 87
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
WO 2002052271	A2	20020704	(200263)*	EN	57

RW: AT BE CH CY DE DK EA ES FI FR GB GR IE IT LU MC NL PT SE TR
 W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK
 DM DZ EC EE ES FI GB GD GE GH HR HU ID IL IN IS JP KE KG KP KR KZ
 LC LK LT LU LV MA MD MK MN MX NO NZ OM PH PL PT RO RU SE SG SI SK
 TJ TM TN TR TT UA US UZ VN YU ZA ZW
 US 2002090652 A1 20020711 (200263)

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2002052271	A2	WO 2001-EP15228	20011221
US 2002090652	A1 Provisional	US 2000-257559P	20001222
	Provisional	US 2001-332965P	20011119
		US 2001-16627	20011210

PRIORITY APPLN. INFO: US 2001-332965P 20011119; US 2000-257559P
 20001222; US 2001-16627 20011210

AN 2002-590607 [63] WPIX

AB WO 200252271 A UPAB: 20021001

NOVELTY - Identifying a differentially expressed protein in two different samples containing a population of proteins comprises performing inverse labeling of proteins.

DETAILED DESCRIPTION - The method of identifying a differentially expressed protein in two different samples containing a population of proteins comprising:

(a) providing two equal protein pools from each of a reference sample and an experimental sample;

(b) labeling the protein pools with a substantially chemically identical isotopically different protein labeling reagent for proteins, where one pool from each of the reference and experimental pools is labeled with an isotopically heavy protein labeling reagent to provide an isotopically heavy-labeled reference and experimental pools, while the remaining reference and experimental pools are labeled with an isotopically light protein labeling reagent to provide an isotopically light-labeled reference and experimental pools;

(c) combining the isotopically light-labeled reference pool with the isotopically heavy-labeled experimental pool to provide a first protein mixture;

(d) combining the isotopically heavy-labeled reference pool with the isotopically light-labeled experimental pool to provide a second protein mixture;

(e) detecting the labeled proteins from each of the two mixtures; and

(f) comparing the labeling pattern obtained for the labeled proteins in the first and second mixtures, where an inverse labeling pattern of a protein in the second mixture compared with the labeling pattern of the protein in the first mixture is indicative of the differentially expressed protein in the two different samples.

USE - The method for performing protein labeling for comparative proteomics called inverse labeling is useful for the rapid identification of marker or target proteins. Comparative analysis of protein profiles from normal and disease states, with or without **drug** treatment, can facilitate the systematic studies of proteins involved in any biological system or disease, revealing new insights into disease mechanism, identifying new targets, providing information on **drug** -action mechanisms and toxicity, or identifying surrogate markers.

ADVANTAGE - The new method of inverse labeling of proteins provides rapid, high throughput, sensitive, reliable and unambiguous identification of various classes of differentially expressed proteins.

Dwg.0/12

L105 ANSWER 15 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
 ACCESSION NUMBER: 2001-355363 [37] WPIX
 DOC. NO. NON-CPI: N2001-258219
 DOC. NO. CPI: C2001-110129
 TITLE: Chemical screening of various chemicals for biological or
 other activity, by performing assay in which chemical(s)
 and/or entities are present in mixture to produce
 outcome, applying static magnetic field, and evaluating.
 DERWENT CLASS: B04 J04 S01 S03
 INVENTOR(S): STAR-LACK, J M; SUGARMAN, J H
 PATENT ASSIGNEE(S): (GLAX) GLAXO GROUP LTD; (GLAX) GLAXO WELLCOME INC
 COUNTRY COUNT: 91
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
WO 2001033257	A1	20010510	(200137)*	EN	35
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TZ UG ZW W: AE AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ DE DK DM EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW					
AU 2001013558	A	20010514	(200149)		
US 6307372	B1	20011023	(200165)		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2001033257	A1	WO 2000-US29982	20001031
AU 2001013558	A	AU 2001-13558	20001031
US 6307372	B1	US 1999-432492	19991102

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2001013558	A Based on	WO 200133257

PRIORITY APPLN. INFO: US 1999-432492 19991102

AN 2001-355363 [37] WPIX

AB WO 200133257 A UPAB: 20010704

NOVELTY - A screening method comprising:

- (a) performing an assay where chemical(s) and/or entities are present in a mixture to produce an outcome in a plate having a plurality of wells;
- (b) applying a static magnetic field (Bo) to the mixture;
- (c) applying RF magnetic pulse(s) to the mixture; and
- (d) measuring and evaluating resulting FID or echo signals to evaluate the outcome of the assay.

DETAILED DESCRIPTION - A screening method comprising:

- (a) providing a plate having a plurality of wells;
- (b) performing an assay in which one or more chemicals and/or entities are present in a mixture to produce an outcome, and where the assay is performed in at least some of the wells of the plate;
- (c) applying a static magnetic field (Bo) to the mixture;
- (d) applying RF magnetic pulse(s) to the mixture; and
- (e) measuring and evaluating resulting FID or echo signals to

evaluate the outcome of the assay.

INDEPENDENT CLAIMS are also included for;

(1) A method of screening comprising: (a) providing a plate having a plurality of wells; (b) combining a test compound with another chemical and/or entity to form a mixture, where the mixture is held within at least one of the wells of the plate, and where the test compound causes a detectable nuclear magnetic resonance signal to be produced that is dependent on the amount of interaction of the test compound with the mixture; (c) applying a static magnetic field (B_0) to the mixture; (d) applying one or more RF magnetic pulses to the mixture; and (e) measuring and evaluating resulting FID or echo signals to obtain information as to whether the test compound is biologically active in the mixture;

(2) A method of screening comprising: (a) providing a plurality of plates that each include multiple wells; (b) introducing a chemical and/or entity into at least some of the wells of each plate; (c) introducing a test compound into wells containing the chemical and/or entity; (d) stacking the plates on top of each other; and (e) inserting the plates into a nuclear magnetic resonance device and screening for any biologically active test compounds;

(3) Multiwell plate comprising: (a) a plate body having a plurality of wells; (b) at least one RF coil disposed within the plate body; and (c) a connector that is adapted to coupled to RF coil to a magnetic resonance imaging system; and

(4) A multiwell plate comprising a plate body having a plurality of wells, where the plate body is constructed of a material selected from a group of materials with desirable magnetic susceptibility properties to minimize spatial distortions and signal losses to facilitate detection of FID signals.

USE - Chemical screening of various chemicals for biological or other activity.

ADVANTAGE - Method gives high throughput chemical screening.

DESCRIPTION OF DRAWING(S) - Figure is a schematic block diagram of a nuclear magnetic resonance system to screen chemicals.

Imaging system 22

Magnet 24

computer 26

Gradient amplifier 28

gradient coils 30

RF coils 32

Transmitter 34

Multi-well plates 36

Receiver 38

Digitizer 40

Monitor 42

Dwg.2/12

*they mean
H₂O*

L105 ANSWER 16 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
 ACCESSION NUMBER: 2001-300472 [31] WPIX
 DOC. NO. CPI: C2001-092328
 TITLE: New **microcluster** liquid, useful for delivering hydration, oxygenation or nutritional agents or medications, produced by subjecting liquid to cavitation and reduced pressure.
 DERWENT CLASS: B07
 INVENTOR(S): HOLLOWAY, M A; HOLLOWAY, W D
 PATENT ASSIGNEE(S): (BIOH-N) BIO HYDRATION RES LAB INC
 COUNTRY COUNT: 95
 PATENT INFORMATION:

PATENT NO KIND DATE WEEK LA PG

 WO 2001030754 A2 20010503 (200131)* EN 43
 RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ
 NL OA PT SD SE SL SZ TZ UG ZW
 W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CR CU CZ DE DK DM
 DZ EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC
 LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PL PT RO RU SD SE
 SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW
 AU 2001030779 A 20010508 (200149)
 BR 2000015223 A 20020618 (200249)
 EP 1237578 A2 20020911 (200267) EN
 R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT
 RO SE SI
 KR 2002072276 A 20020914 (200311)
 US 6521248 B1 20030218 (200317)
 JP 2003514646 W 20030422 (200336) 48
 CN 1399559 A 20030226 (200337)

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2001030754	A2	WO 2000-US41670	20001026
AU 2001030779	A	AU 2001-30779	20001026
BR 2000015223	A	BR 2000-15223	20001026
EP 1237578	A2	WO 2000-US41670	20001026
		EP 2000-990975	20001026
		WO 2000-US41670	20001026
KR 2002072276	A	KR 2002-705363	20020426
US 6521248	B1 Provisional	US 1999-161546P	19991026
		US 2000-698537	20001026
JP 2003514646	W	WO 2000-US41670	20001026
		JP 2001-533109	20001026
CN 1399559	A	CN 2000-816223	20001026

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2001030779	A Based on	WO 200130754
BR 2000015223	A Based on	WO 200130754
EP 1237578	A2 Based on	WO 200130754
JP 2003514646	W Based on	WO 200130754

PRIORITY APPLN. INFO: US 1999-161546P 19991026; US 2000-698537
 20001026

AN 2001-300472 [31] WPIX
 AB WO 200130754 A UPAB: 20011129

NOVELTY - Producing (M1) a micro-cluster liquid comprising:

- (a) subjecting a liquid to cavitation such that dissolved entrained gases in the liquid form a number of cavitation bubbles; and
- (b) subjecting the liquid to reduced pressure, which causes breakage of large molecule matrices into smaller liquid molecule matrices, producing a micro-cluster liquid, is new.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

- (1) producing (M2) a micro-cluster liquid produced comprising:
 - (a) subjecting a liquid to a pressure sufficient to pressurize the liquid;
 - (b) emitting the pressurized liquid such that a continuous stream of

liquid is created;

(c) subjecting the continuous stream of liquid to a multiple rotational vortex having a partial vacuum pressure such that dissolved entrained gases in the liquid form a number of cavitation bubbles; and

(d) subjecting the liquid containing the cavitation bubbles to a reduced pressure, where the cavitation bubbles implode or explode causing shock waves that break large liquid molecule matrices into smaller liquid molecule matrices, thereby producing a micro-cluster liquid;

(2) a micro-cluster liquid or water produced by M1 or M2;

(3) a composition comprising a micro-cluster water having a conductivity of about 3.0 - 4.0 micromhos/cm;

(4) a composition comprising a micro-cluster water having a Fourier transform infrared (FTIR) spectrophotometric pattern comprising a major sharp feature at about 2650 wave numbers;

(5) a composition comprising a micro-cluster water having a vapor pressure between 40 - 70 degrees C as determined by thermogravimetric analysis;

(6) a composition comprising a micro-cluster water having an 170 nuclear magnetic resonance (NMR) peak shift of at least about +30 Hertz relative to reverse osmosis water; and

(7) modulating a cellular performance comprising contacting a cell with a micro-cluster water.

USE - The microcluster water is used to deliver hydration, oxygenation, or agents, such as nutritional agents or medications.

ADVANTAGE - The microcluster water increases overall cellular performance and exchanging liquids in the cell within minutes of consumption.

Dwg.0/7

L105 ANSWER 17 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
 ACCESSION NUMBER: 2002-017002 [02] WPIX
 CROSS REFERENCE: 1998-610081 [51]; 2001-181394 [08]
 DOC. NO. NON-CPI: N2002-013679
 DOC. NO. CPI: C2002-004714
 TITLE: Isotopically modified topical composition for improving skin appearance and texture, comprises cosmetic material mixed with liquid light transport modifier.
 DERWENT CLASS: B06 D21 P34 S05
 INVENTOR(S): BERRY, M J; YAVITZ, E Q
 PATENT ASSIGNEE(S): (NATU-N) NATURAL VISION CENT INC
 COUNTRY COUNT: 1
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
US 6312450	B1	20011106	(200202)*		9

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
US 6312450	B1 CIP of	US 1997-858967	19970520
		US 1999-379183	19990823

FILING DETAILS:

PATENT NO	KIND	PATENT NO
US 6312450	B1 CIP of	US 6009876

PRIORITY APPLN. INFO: US 1999-379183 19990823; US 1997-858967
19970520

AN 2002-017002 [02] WPIX
CR 1998-610081 [51]; 2001-181394 [08]
AB US 6312450 B UPAB: 20020109

NOVELTY - An isotopically modified topical composition, comprising a mixture of cosmetic or cosmeceutical material, and a liquid light transport modifier, is new. The light transport modifier is readily absorbed by an epidermal layer of mammalian skin to permit passage of infrared energy through the epidermal layer at reduced energy absorption.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

(1) using infrared energy to improve the appearance of skin of an individual comprising:

(a) selecting an isotopically modified substance that permits passage of a desired radiation in the infrared region through the epidermis;

(b) applying the isotopically modified substance to an area of the epidermis; and

(c) heating the papillary dermis layer between the epidermis and the reticular dermis at the area in order to stimulate the release of factors that promote new collagen growth; and

(2) improving the effectiveness of a cosmetic or cosmeceutical composition, comprising:

(a) providing the cosmetic or cosmeceutical composition; and

(b) isotopically modifying at least one of the chemical elements contained in the cosmetic or cosmeceutical composition to alter the energy absorption characteristics and pharmacokinetic properties of the composition.

USE - For improving the appearance and texture of individual's skin epidermis.

ADVANTAGE - The composition reduces absorption of certain types of electromagnetic energy that strike the epidermis. The light transport modifier is designed to displace naturally occurring **water** within that portion, thus resulting in a reduced heat buildup in that portion. The epidermis remains intact with less chance of infection, decrease redness and loss of body fluid, and short healing time.
Dwg.0/4

L105 ANSWER 18 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN

ACCESSION NUMBER: 2001-435706 [47] WPIX

DOC. NO. CPI: C2001-132030

TITLE: Manufacture of **water** for cosmetics, involves passing raw **water** through salt form and/or regeneration type ion exchange resin, and adjusting nuclear magnetic resonance signal half width value of **170** in **water**.

DERWENT CLASS: A91 B07 D15 D21

PATENT ASSIGNEE(S): (JAOR) ORGANO CORP

COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
JP 2001096272 A		20010410	(200147)*		4

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE

WELLS 09/744,550

JP 2001096272 A

JP 1999-274078 19990928

PRIORITY APPLN. INFO: JP 1999-274078 19990928

AN 2001-435706 [47] WPIX

AB JP2001096272 A UPAB: 20010822

NOVELTY - The method involves passing raw **water** through a salt form ion exchange resin or a mixed bed of salt form and regeneration type ion exchange resin. The nuclear magnetic resonance signal half width value of **170** in **water**, is adjusted.

DETAILED DESCRIPTION - An INDEPENDENT CLAIM is also included for the **water** treatment method. The salt form ion exchange resin is a carbonate and/or bicarbonate type anion exchange resin.

USE - For dilution of concentrated liquids, for drinking **water**, cosmetics, **drugs**, brewing and juice production (all claimed).

ADVANTAGE - **Water** with reduced **170** nuclear magnetic resonance signal half width value, is manufactured stably and efficiently.

Dwg.0/0

L105 ANSWER 19 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN

ACCESSION NUMBER: 2000-255683 [22] WPIX

CROSS REFERENCE: 1998-119933 [11]

DOC. NO. CPI: C2000-077937

TITLE: Microclustered **water** useful for preparing medicaments for the treatment of e.g. **burns**, pain, diabetes and viral infections.

DERWENT CLASS: B07 C07 D16 J04

INVENTOR(S): LORENZEN, L H

PATENT ASSIGNEE(S): (LORE-I) LORENZEN L H

COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
US 6033678	A	20000307	(200022)*		8

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
US 6033678	A	CIP of	US 1990-463988 19900112
		Cont of	US 1991-670032 19910315
		Cont of	US 1992-990357 19921215
		Cont of	US 1994-208799 19940309
			US 1997-984777 19971204

FILING DETAILS:

PATENT NO	KIND	PATENT NO
US 6033678	A	Cont of US 5711950

PRIORITY APPLN. INFO: US 1991-670032 19910315; US 1990-463988 19900112; US 1992-990357 19921215; US 1994-208799 19940309; US 1997-984777 19971204

AN 2000-255683 [22] WPIX

CR 1998-119933 [11]

AB US 6033678 A UPAB: 20000508

NOVELTY - A process for producing microclustered water comprising boiling water, passing the steam across a magnetic field, condensing the steam and adding a stabilizer and pressure to the condensed steam, is new.

DETAILED DESCRIPTION - A process for producing microclustered water comprises:

- (a) boiling water;
- (b) passing the steam across a magnetic field;
- (c) condensing the steam at a temperature greater than 0 deg. C in the presence of light in the far infra-red to ultraviolet spectrum range to produce condensed steam;
- (d) adding a stabilizer (metasilicate salt) and less than 1% of a dietary supplement template;
- (e) exposing the condensed steam to a pressure greater than 1 atmosphere; and
- (f) depressurizing the condensed steam to produce the microclustered water.

The microclustered water produces an 170 nuclear magnetic resonance (NMR) signal less than 115 Hz, has a conductivity of at least 3.7 psi s/cm and a surface tension of less than 61 dynes/cm.

USE - The microclustered water provides a means of treating abnormal states in a living organism by using a template which has activity in treating the abnormal state. The method is especially useful for treating burns, pain, diabetes and viral infections.

Dwg.0/2

L105 ANSWER 20 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
 ACCESSION NUMBER: 2000-658426 [64] WPIX
 DOC. NO. CPI: C2000-199453
 TITLE: New liposome, used in e.g. cosmetics and medicines comprises object substance and amphoteric compound e.g. phospholipid.
 DERWENT CLASS: B04 D21
 PATENT ASSIGNEE(S): (HATT-I) HATTORI T
 COUNTRY COUNT: 1
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
JP 2000229815 A		20000822	(200064)*		8

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2000229815 A		JP 1999-28910	19990205

PRIORITY APPLN. INFO: JP 1999-28910 19990205

AN 2000-658426 [64] WPIX

AB JP2000229815 A UPAB: 20001209

NOVELTY - A liposome (I), obtained by mixing water having 90 Hz or less of half value of 170-NMR signal, amphoteric substance and object substance, is new.

DETAILED DESCRIPTION - A liposome (I), obtained by mixing water having 90 Hz or less of half value of 170-NMR signal, amphoteric substance and phospholipid is new.

USE - (I) is used as material for cosmetics and medicines.

Dwg.0/0

L105 ANSWER 21 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
 ACCESSION NUMBER: 2000-091849 [08] WPIX
 DOC. NO. NON-CPI: N2000-071931
 DOC. NO. CPI: C2000-026656
 TITLE: Pure **water** and preparation of pure **water** - for use in **parenteral** injections.
 DERWENT CLASS: B07 D15 D21 P81 U11
 PATENT ASSIGNEE(S): (HATT-I) HATTORI T
 COUNTRY COUNT: 1
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
JP 11333498	A	19991207	(200008)*		11

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 11333498	A	JP 1998-145319	19980527

PRIORITY APPLN. INFO: JP 1998-145319 19980527

AN 2000-091849 [08] WPIX

AB JP 11333498 A UPAB: 20000215

NOVELTY - Pure **water** having electric conductivity of up to 1 mS/cm, preferably up to 0.2 mS/cm, and a half value width of 170 -NMR of up to 69 Hz is new. DETAILED DESCRIPTION - An independent claim is also included for preparation of the above-claimed pure **water**, which includes (1) a process of allowing **water** to pass through a reverse osmosis membrane and (2) a process of allowing **water** to pass through an ion exchange membrane and/or an ion exchange resin. The preparation preferably includes an additional process of allowing **water** to pass through an ultrafilter; more preferably a process of magnetisation is also included.

USE - The pure **water** can be used in **parenteral** injections., eye drops, and cosmetic solutions.

ADVANTAGE - The pure **water** obtained has high activity as **water** and contains almost no impurities.

Dwg.0/1

L105 ANSWER 22 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN
 ACCESSION NUMBER: 1998-119933 [11] WPIX
 CROSS REFERENCE: 2000-255683 [19]
 DOC. NO. NON-CPI: N1998-095456
 DOC. NO. CPI: C1998-039353
 TITLE: Preparation of micro-clustered **water** from starting **water** - by boiling **water**, passing through magnetic field, exposing to light, condensing, adding stabiliser, adding **yeast** cells or anti-viral agent, exposing to high pressure and depressurising.
 DERWENT CLASS: B07 C04 C07 D15 D16 H06 J04 X25
 INVENTOR(S): LORENZEN, L H
 PATENT ASSIGNEE(S): (LORE-I) LORENZEN L H
 COUNTRY COUNT: 1
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
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 US 5711950 A 19980127 (199811)* 6

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
US 5711950	A	CIP of	US 1990-463988 19900112
		Cont of	US 1991-670032 19910315
		Cont of	US 1992-990357 19921215
			US 1994-208799 19940309

PRIORITY APPLN. INFO: US 1991-670032 19910315; US 1990-463988
 19900112; US 1992-990357 19921215; US
 1994-208799 19940309

AN 1998-119933 [11] WPIX

CR 2000-255683 [19]

AB US 5711950 A UPAB: 20000508

Preparation of microclustered **water** from a starting **water** comprises: (a) Boiling the starting **water** to produce steam; (b) passing the steam across a magnetic field; (c) exposing the steam to light of wavelength 610 nm - 1 mm; (d) condensing the steam at a temperature > 0 deg. C, giving condensed steam; (e) adding at least one stabiliser, comprising a metasilicate salt, to the condensed steam; (f) adding **yeast** cells or an anti-viral agent, of concentration at most 1 %, to the condensed steam; (g) exposing the condensed steam to a pressure > 1 atmosphere; and (h) depressurising the condensed steam producing microclustered **water**. The microclustered **water** produces an 170 nuclear magnetic resonance (NMR) signal of < 115 Hz, has a conductivity of at least 3.7 mu s/cm, and has a surface tension of > 61 dynes/cm. Steps (e) and (f) may be reversed.

USE - The microclustered **water** product is used in medicaments for the treatment of viral infections, and in medicaments for promotion of growth of living organisms. The process can also be used to produce medicaments for treating **burns**, pain, diabetes, and also catalysts and agricultural products.
 Dwg.0/2

L105 ANSWER 23 OF 23 WPIX COPYRIGHT 2003 THOMSON DERWENT on STN

ACCESSION NUMBER: 1991-007934 [02] WPIX

DOC. NO. NON-CPI: N1991-006206

DOC. NO. CPI: C1991-003520

TITLE: Magnetic resonance **tomography** and localised spectroscopy - has gp. of impulse sequences, contrast chemicals and data analysis to improve resolution.

DERWENT CLASS: B02 E12 J04 P31 S01 S03 S05 T01

INVENTOR(S): KIMMICH, R; ROMMEL, E

PATENT ASSIGNEE(S): (KIMM-I) KIMMICH R; (ROMM-I) ROMMEL E

COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
DE 3919052	A	19910103 (199102)*			
DE 3919052	C2	19930624 (199325)			12

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
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DE 3919052	A	DE 1989-3919052	19890610
DE 3919052	C2	DE 1989-3919052	19890610

PRIORITY APPLN. INFO: DE 1989-3919052 19890610

AN: 1991-007934 [02] WPIX

AB DE 3919052 A UPAB: 19930928

In a nuclear magnetic resonance system, the signal acquisition period is chosen in relation to the spin locking period of the magnetising. This allows the formation or influence of picture contrast or characteristic resonance by :- (a) one of the two variables of the rotating coordinates of the spin lattice relaxation time; (b) the frequency dependence of one of these two variables. (c) The susceptibility dependence of one of these two variables.

Pref the spin locking is at or near resonance where the effective magnetic field is aligned with the magnetising to be locked or, off resonance to reduce power demand for the high frequency RF field but allow misalignment of the effective field from the field to be locked.

USE/ADVANTAGE - In nuclear magnetic resonance based **tomography**, localised relaxometry and localised spectroscopy. Previously inaccessible material characteristics can be identified. When contrast intensifiers are used the doses can be considerably reduced. Information can be taken as contrast or volume selection data measurements. No additional measurements are necessary in normal areas. @ (12pp Dwg.No.1/7)@

ABEQ DE 3919052 C UPAB: 19931116

In a process for **tomography**, partic. for medical applications, based on magnetic resonance imaging, signals are recorded in a spin-locking condition or several effective frequencies and image contrast is represented by the difference between the signals. The effective field during spin-locking differs from the direction of magnetisation.

The process is used with electron paramagnetic contrast media, pref. Mn-tetra-phenyl-(p-sulphonatophenyl) -porphyrin, or diamagnetic media, pref. ¹⁷O-enriched cpds. e.g. **water**.

ADVANTAGE - Reduced contrast media requirement, improved tissue characterisation data.
Dwg. 1/7

=> file home

FILE 'HOME' ENTERED AT 17:29:23 ON 21 JUL 2003

WELLS 09/744,550

=> d que 110

L9 43498 SEA FILE=CAPLUS ABB=ON PLU=ON CYSTEINE/OBI
 L10 2 SEA FILE=CAPLUS ABB=ON PLU=ON L9(L)(33S OR SULFUR-33)

=> d que 118

L16 49772 SEA FILE=CAPLUS ABB=ON PLU=ON (THIOL OR SULFHYDR?)/OBI
 L17 6 SEA FILE=CAPLUS ABB=ON PLU=ON L16 AND (33S OR SULFUR-33)
 L18 3 SEA FILE=CAPLUS ABB=ON PLU=ON L17 AND (DISULFIDES OR
 SHIELDING OR COENZYME)/TI

=> d que 121

L19 80329 SEA FILE=CAPLUS ABB=ON PLU=ON (THIOL OR ?SULFHYDRYL?)
 L21 3 SEA FILE=CAPLUS ABB=ON PLU=ON L19(P)(33S OR SULFUR-33)

=> s 110 or 118 or 121

L53 6 L10 OR L18 OR L21

=> d ibib abs hitrn ind 1-6

L53 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:263972 CAPLUS

DOCUMENT NUMBER: 138:398030

TITLE: Coenzyme B Induced Coordination of
 Coenzyme M via Its Thiol Group to
 Ni(I) of F430 in Active Methyl-Coenzyme M
 Reductase

AUTHOR(S): Finazzo, Cinzia; Harmer, Jeffrey; Bauer, Carsten;
 Jaun, Bernhard; Duin, Evert C.; Mahlert, Felix;
 Goenrich, Meike; Thauer, Rudolf K.; Van Doorslaer,
 Sabine; Schweiger, Arthur
 CORPORATE SOURCE: Physical Chemistry and Organic Chemistry, ETH Zurich,
 Zurich, CH-8093, Switz.

SOURCE: Journal of the American Chemical Society (2003),
 125(17), 4988-4989

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Methyl-coenzyme M reductase (MCR) catalyzes the reaction of
 methyl-coenzyme M (CH₃-S-CoM) with coenzyme B (HS-CoB) to methane and
 CoM-S-S-CoB. At the active site, it contains the nickel porphinoide F430,
 which has to be in the Ni(I) oxidn. state for the enzyme to be active.
 How the substrates interact with the active site Ni(I) has remained
 elusive. We report here that coenzyme M (HS-CoM), which is a reversible
 competitive inhibitor to methyl-coenzyme M, interacts with its
 thiol group with the Ni(I) and that for interaction the
 simultaneous presence of coenzyme B is required. The evidence is based on
 X-band continuous wave EPR and Q-band hyperfine sublevel correlation
 spectroscopy of MCR in the red2 state induced with 33S-labeled
 coenzyme M and unlabeled coenzyme B.

CC 7-3 (Enzymes)

ST sulfhydryl group nickel cofactor F430 methyl coenzyme reductase

IT Enzyme functional sites

(active; coenzyme B induced coordination of coenzyme M via its
 thiol group to Ni(I) of F430 in active Me-coenzyme M reductase)

IT Sulfhydryl group

(coenzyme B induced coordination of coenzyme M via its thiol

- group to Ni(I) of F430 in active Me-coenzyme M reductase)
- IT Reduction
(enzymic; coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
- IT 74-82-8, Methane, biological studies 7440-02-0, Nickel, biological studies 45127-11-5, Coenzyme M 53501-90-9, Methyl-coenzyme M 73145-13-8, Cofactor F430 104302-77-4, Coenzyme B
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
- IT 53060-41-6, Methyl-coenzyme M reductase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
- IT 532427-72-8P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
- IT 4263-52-9 532427-66-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
- IT 532427-67-1P 532427-70-6P 532427-71-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(coenzyme B induced coordination of coenzyme M via its **thiol** group to Ni(I) of F430 in active Me-coenzyme M reductase)
- REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:196114 CAPLUS

DOCUMENT NUMBER: 139:49012

TITLE: Coenzyme M binds to a [4Fe-4S] cluster in the active site of heterodisulfide reductase as deduced from EPR studies with the [33S]coenzyme M-treated enzyme

AUTHOR(S): Duin, Evert C.; Bauer, Carsten; Jaun, Bernhard; Hedderich, Reiner

CORPORATE SOURCE: Max-Planck-Institut für Terrestrische Mikrobiologie, Marburg, D-35043, Germany

SOURCE: FEBS Letters (2003), 538(1-3), 81-84
CODEN: FEBLAL; ISSN: 0014-5793

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Heterodisulfide reductase (Hdr) from methanogenic Archaea catalyzes the reversible redn. of the heterodisulfide (CoM-S-S-CoB) of the methanogenic **thiol** coenzymes, coenzyme M (CoM-SH) and coenzyme B (CoB-SH). Upon reaction of the oxidized enzyme with CoM-SH a unique paramagnetic species is formed, which has been shown to be due to a novel type of [4Fe-4S]³⁺ cluster. In this work, it was addressed whether CoM-SH is directly attached to this [4Fe-4S] cluster using CoM-33SH as substrate and purified Hdr from Methanothermobacter marburgensis and Methanosarcina barkeri. With both enzymes treatment with CoM-33SH in the presence of duroquinone as an oxidant resulted in a significant broadening of the ESR spectrum as compared to CoM-SH as substrate. The signal broadening resulted from an unresolved anisotropic hyperfine coupling between the 33S nucleus and the paramagnetic center. The results provide

compelling evidence for a direct binding of CoM-SH to the [4Fe-4S] cluster in the active site of the enzyme.

CC 7-3 (Enzymes)

ST coenzyme M binding iron sulfur cluster heterodisulfide reductase

IT Iron-sulfur clusters (protein)

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(coenzyme M binds to [4Fe-4S] cluster in active site of heterodisulfide reductase)

IT Enzyme functional sites

(cofactor-binding; coenzyme M binds to [4Fe-4S] cluster in active site of heterodisulfide reductase)

IT 7439-89-6D, Iron, sulfur clusters 7704-34-9D, Sulfur, iron clusters
45127-11-5, Coenzyme M 104302-77-4, Coenzyme B

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(coenzyme M binds to [4Fe-4S] cluster in active site of heterodisulfide reductase)

IT 116515-35-6, Heterodisulfide reductase

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
(Biological study)

(coenzyme M binds to [4Fe-4S] cluster in active site of heterodisulfide reductase)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:67270 CAPLUS

DOCUMENT NUMBER: 128:175199

TITLE: Ab initio calculation of NMR properties (shielding and electric field gradient) of
33S in sulfur compounds

AUTHOR(S): Bagno, Alessandro

CORPORATE SOURCE: Dipartimento di Chimica Organica, Universita di
Padova, Padua, 35131, Italy

SOURCE: THEOCHEM (1997), 418(2-3), 243-255

CODEN: THEODJ; ISSN: 0166-1280

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Chem. shieldings of the S nucleus were calcd. with the GIAO method for a wide range of org. and inorg. S compds., using the 6-311++G(2d,2p) basis set. The resulting data, including calcd. elec. field gradients, are compared with other theor. results and exptl. 33S NMR chem. shifts and line widths; with a resulting relation, joined to calcd. elec. field gradients at the nuclei, can be employed for predicting the chem. shift and line width of hitherto undetected signals. There is no general relation between 33S shielding and electronic charge at S.

CC 77-7 (Magnetic Phenomena)

ST NMR sulfur 33 compd; EFG sulfur 33
; nuclear shielding sulfur 33

IT Electric field gradient

GIAO (gauge invariant atomic orbital)

NMR (nuclear magnetic resonance)

Nuclear shielding

(ab initio calcn. of NMR properties of sulfur-33 in sulfur compds.)

IT 66-27-3, Methyl methanesulfonate 67-68-5, Dimethylsulfoxide, properties
67-71-0 74-93-1, Methane thi 1, properties 75-15-0, Carbon
disulfide, properties 75-18-3, Dimethyl sulfide 75-75-2,
Methanesulfonic acid 110-02-1, Thiophene 288-47-1, Thiazole
302-04-5, Thiocyanate, properties 463-58-1, Carbon oxide sulfide (COS)

556-61-6 556-64-9, Methyl thiocyanate 624-92-0, Dimethyl disulfide
 666-15-9 676-84-6, Trimethyl sulfonium 758-16-7 1534-08-3
 2168-84-5 2551-62-4, Sulfur fluoride (SF₆) 3086-29-1, Trimethyl
 sulfonium chloride 3144-09-0, Methyl sulfonamide 3658-80-8, Dimethyl
 trisulfide 4291-05-8 4756-05-2, Thioacetone 7446-09-5, Sulfur
 dioxide, properties 7446-11-9, Sulfur trioxide, properties 7719-09-7,
 Sulfinyl dichloride 7783-06-4, Dihydrogen sulfide, properties
 7783-60-0, Sulfur tetrafluoride 7791-25-5, Sulfonyl chloride
 10544-50-0, Sulfur (S₈), properties 14257-58-0, **Sulfur-**
33, properties 14265-45-3, Sulfite 14383-50-7, Thiosulfate
 (S₂O₃²⁻) 14808-79-8, Sulfate, properties 14844-07-6, Dithionite
 15035-72-0, Hydrogen sulfide (HS⁻) 15644-49-2, Carbonotrithioate
 16053-58-0, Methanesulfonic acid, ion(1-) 18155-21-0, Hydrogen sulfide
 ion (HS⁻) 18496-25-8, Sulfide 18649-16-6, Methanesulfinamide
 18683-23-3, Protonated methanethiol 21119-13-1 63056-18-8 68226-03-9
 85504-08-1, Methanesulfenamide 202993-74-6, Sulfonium chloride ((SH₃)C⁺)
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PROC (Process)

(ab initio calcn. of NMR properties of **sulfur-33** in
 sulfur compds.)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L53 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:404800 CAPLUS

DOCUMENT NUMBER: 87:4800

TITLE: Spectroscopic methods for the study of organic
thiols, sulfides and **disulfides**

AUTHOR(S): Jung, Guenther; Ottnad, Michael

CORPORATE SOURCE: Chem. Inst., Univ. Tuebingen, Tuebingen, Fed. Rep.
 Ger.

SOURCE: Themen Chem. Schwefels (1975), 167-91. Editor(s):
 Maas, Klaus. Huethig: Heidelberg, Ger.

CODEN: 35HPAM

DOCUMENT TYPE: Conference; General Review

LANGUAGE: German

AB A review with 130 refs.

CC 22-0 (Physical Organic Chemistry)

ST review spectra sulfur org; **thiol** org spectra review; sulfide org
 spectra review; disulfide org spectra review

IT Spectra

(disulfides, sulfides, and **thiols**)

IT Circular dichroism

Electron spin resonance

Infrared spectra

Optical rotatory dispersion

Photoelectron spectroscopy

Ultraviolet and visible spectra

(of org. sulfur compds.)

IT Nuclear magnetic resonance

(of **sulfur-33**, of org. sulfur compds.)

IT Disulfides

Sulfides, properties

Thiols, properties

RL: PRP (Properties)

(spectra of)

L53 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1977:155929 CAPLUS

DOCUMENT NUMBER: 86:155929

TITLE: Nuclear coupling of **sulfur-33** and the nature of free radicals in irradiated crystals of N-acetyl-L-cysteine

AUTHOR(S): Hadley, Joseph H., Jr.; Gordy, Walter

CORPORATE SOURCE: Dep. Phys., Georgia State Univ., Atlanta, GA, USA

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1977), 74(1), 216-20
CODEN: PNASA6; ISSN: 0027-8424

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Hyperfine structure due to ³³S in its natural abundance of 0.76% was measured in the ESR of free radicals produced by x-irradn. of single crystals of N-acetyl-L-cysteine at 7.7 K. Radicals produced at 77 K with principal g values of 1.990, 2.006, and 2.214 are monosulfide radicals with the 3p unpaired electron d. of 0.70 on the S. They are neg. charged mols. RCH₂S-H or neutral RCH₂SH₂ radicals in which 90% of the spin d. of the captured electron is concd. in a d-p hybrid orbital on the S. At 300 K, these, as well as the C-centered radicals produced at the lower temp., are converted to neutral disulfide radicals RCH₂SS like those obsd. in irradiated cystine.

CC 34-2 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22

ST acetylcysteine irradiation ESR; cysteine acetyl ESR

IT Radicals, properties
RL: PRP (Properties)
(ESR of sulfur-33, in irradiated crystals of acetylcysteine)

IT Electron spin resonance
(of sulfur 33, in irradiated crystals of acetylcysteine)

IT Electron spin resonance
(of sulfur-33 in irradiated crystals of acetylcysteine)

IT 616-91-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(irradiation of, free radicals in, ESR of)

IT 14257-58-0, properties
RL: RCT (Reactant); RACT (Reactant or reagent)
(nuclear coupling of, in ESR of irradiated acetylcysteine)

L53 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:31403 CAPLUS

DOCUMENT NUMBER: 84:31403

TITLE: Nuclear coupling of **sulfur-33** and the nature of free radicals in irradiated crystals of cysteine hydrochloride and N-acetyl methionine

AUTHOR(S): Hadley, Joseph H., Jr.; Gordy, Walter

CORPORATE SOURCE: Dep. Phys., Georgia State Univ., Atlanta, GA, USA

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1975), 72(9), 3486-90
CODEN: PNASA6; ISSN: 0027-8424

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The ³³S hyperfine structure was obsd. in the ESR of irradiated crystals of cysteine.HCl.H₂O and of N-acetyl-DL-methionine. In both substances the free radicals that are stable at room temp. are disulfide radicals, RCH₂SS.

CC 34-2 (Synthesis of Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 22

ST ESR cysteine methionine radical; radical irradiation sulfur

IT Electron spin resonance
(of cysteine hydrochloride and acetylmethionine, free radicals in relation to)

WELLS 09/744,550

IT Spin, nuclear coupling
(of labeled sulfur, in cysteine and methionine)
IT 1115-47-5 7048-04-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(irradn. of crystals of, ESR of)

Search for ¹⁴N-H biological cpds

WELLS 09/744,550

=> d que 157

L55	2564	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	NITROGEN ISOTOPES/CT
L56	27	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L55 AND ISOLEUCINE
L57	2	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L56 AND 14N <i>2 cites</i>

=> d que 160

L55	2564	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	NITROGEN ISOTOPES/CT
L58	254	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L55 AND RELAX?
L59	78	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L58 AND AMINO ACID
L60	2	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L59 AND 14N <i>2 cites</i>

=> d que 166

L55	2564	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	NITROGEN ISOTOPES/CT
L63	77	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L55 AND (14N OR NITROGEN-14)
L64	20	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L63 AND (MAGNETIC OR NMR)
L65	5	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L64 AND HYDROGEN
L66	3	SEA	FILE=MEDLINE	ABB=ON	PLU=ON	L65 NOT (ALGAE OR AMMONIA)/TI <i>3 cites</i>

=> s 157 or 160 or 166

L67 5 L57 OR L60 OR L66 *5 cites total*

=> d ibib abs ind 1-5

L67 ANSWER 1 OF 5 MEDLINE on STN
 ACCESSION NUMBER: 1999311318 MEDLINE
 DOCUMENT NUMBER: 99311318 PubMed ID: 10382309
 TITLE: Application of amino acid type-specific
 1H- and 14N-labeling in a 2H-, 15N-labeled
 background to a 47 kDa homodimer: potential for NMR
 structure determination of large proteins.
 AUTHOR: Kelly M J; Krieger C; Ball L J; Yu Y; Richter G; Schmieder
 P; Bacher A; Oschkinat H
 CORPORATE SOURCE: Forschungsinstitut fur Molekulare Pharmakologie, Berlin,
 Germany.. kelly@fmp-berlin.de
 SOURCE: JOURNAL OF BIOMOLECULAR NMR, (1999 May) 14 (1) 79-83.
 Journal code: 9110829. ISSN: 0925-2738.
 PUB. COUNTRY: Netherlands
 DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
 LANGUAGE: English
 FILE SEGMENT: Priority Journals
 ENTRY MONTH: 199907
 ENTRY DATE: Entered STN: 19990730
 Last Updated on STN: 20000303
 Entered Medline: 19990722
 AB NMR investigations of larger macromolecules (> 20 kDa) are
 severely hindered by rapid 1H and 13C transverse relaxation.
 Replacement of non-exchangeable protons with deuterium removes many
 efficient 1H-1H and 1H-13C relaxation pathways. The main
 disadvantage of deuteration is that many of the protons which would
 normally be the source of NOE-based distance restraints are removed. We
 report the development of a novel labeling strategy which is based on
 specific protonation and 14N-labeling of the residues
 phenylalanine, tyrosine, threonine, isoleucine and valine in a
 fully deuterated, 15N-labeled background. This allows the application of
 heteronuclear half-filters, 15N-editing and 1H-TOCSY experiments to select
 for particular magnetization transfer pathways. Results from

investigations of a 47 kDa dimeric protein labeled in this way demonstrated that the method provides useful information for the structure determination of large proteins.

CT Check Tags: Support, Non-U.S. Gov't

Amino Acid Sequence

Amino Acids

Deuterium

Dimerization

Hydrogen

Molecular Weight

Nitrogen

Nitrogen Isotopes

Nuclear Magnetic Resonance, Biomolecular: MT, methods

*Oligopeptides: CH, chemistry

Protein Conformation

*Proteins: CH, chemistry

RN 1333-74-0 (Hydrogen); 7727-37-9 (Nitrogen); 7782-39-0 (Deuterium)

CN 0 (Amino Acids); 0 (Nitrogen Isotopes); 0 (Oligopeptides); 0 (Proteins)

L67. ANSWER 2 OF 5

MEDLINE on STN

ACCESSION NUMBER: 97144788 MEDLINE

DOCUMENT NUMBER: 97144788 PubMed ID: 8990521

TITLE: 15N conservation in the metabolic conversion of **isoleucine** to alloisoleucine in the rat.

AUTHOR: Mamer O A; Lepine F L

CORPORATE SOURCE: Biomedical Mass Spectrometry Unit, McGill University, Montreal, Quebec, Canada.

SOURCE: JOURNAL OF MASS SPECTROMETRY, (1996 Dec) 31 (12) 1382-8. Journal code: 9504818. ISSN: 1076-5174.

PUB. COUNTRY: ENGLAND: United Kingdom

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 199702

ENTRY DATE: Entered STN: 19970305

Last Updated on STN: 19970305

Entered Medline: 19970218

AB 15N,13C6-L-**Isoleucine** was given by stomach tube to a pair of rats and the urine excreted over the following 6 h period was collected. The urinary amino acid fraction showed that the majority of the L-alloisoleucine produced from the labeled **isoleucine** was formed with the 15N label intact. This fails to support the commonly held supposition that L-**isoleucine** and L-alloisoleucine interconversion occurs through the reversible enolization of the 2-keto-3-methylvaleric acids formed by their transamination. In contrast to 15N label conservation in L-alloisoleucine, the majority of the 15N in the administered L-**isoleucine** underwent exchange with 14N.

CT Check Tags: Animal; Male

Biotransformation

Indicators and Reagents

***Isoleucine**: PK, pharmacokinetics

Isoleucine: UR, urine

Mass Fragmentography

*Nitrogen: ME, metabolism

Nitrogen Isotopes

Organosilicon Compounds

Rats

Rats, Sprague-Dawley

Trifluoroacetic Acid: AA, analogs & derivatives

RN 73-32-5 (Isoleucine); 76-05-1 (Trifluoroacetic Acid); 7727-37-9 (Nitrogen); 77377-52-7 (N-methyl-N-(tert-butyldimethylsilyl)trifluoroacetamide)

CN 0 (Indicators and Reagents); 0 (Nitrogen Isotopes); 0 (Organosilicon Compounds)

L67 ANSWER 3 OF 5

MEDLINE on STN

ACCESSION NUMBER: 95005911 MEDLINE

DOCUMENT NUMBER: 95005911 PubMed ID: 7921674

TITLE: Assignment of amino acid type in 1H-15N correlation spectra by labeling with 14N-amino acids.

AUTHOR: Shortle D

CORPORATE SOURCE: Department of Biological Chemistry, Johns Hopkins University School of Medicine, Baltimore, Maryland 21205.

CONTRACT NUMBER: GM34171 (NIGMS)

SOURCE: JOURNAL OF MAGNETIC RESONANCE. SERIES B, (1994 Sep) 105 (1) 88-90.

Journal code: 9309764. ISSN: 1064-1866.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 199411

ENTRY DATE: Entered STN: 19941222

Last Updated on STN: 19941222

Entered Medline: 19941116

CT Check Tags: Support, U.S. Gov't, P.H.S.

*Amino Acids

Amino Acids: AN, analysis

Hydrogen

*Magnetic Resonance Spectroscopy

Micrococcal Nuclease: CH, chemistry

Nitrogen

Nitrogen Isotopes

RN 1333-74-0 (Hydrogen); 7727-37-9 (Nitrogen)

CN 0 (Amino Acids); 0 (Nitrogen Isotopes); EC 3.1.31.1 (Micrococcal Nuclease)

L67 ANSWER 4 OF 5

MEDLINE on STN

ACCESSION NUMBER: 94151290 MEDLINE

DOCUMENT NUMBER: 94151290 PubMed ID: 8108380

TITLE: A comparison of 15N NMR relaxation measurements with a molecular dynamics simulation: backbone dynamics of the glucocorticoid receptor DNA-binding domain.

AUTHOR: Eriksson M A; Berglund H; Hard T; Nilsson L

CORPORATE SOURCE: Center for Structural Biochemistry (CSB), Karolinska Institute, NOVUM, Huddinge, Sweden.

SOURCE: PROTEINS, (1993 Dec) 17 (4) 375-90.

Journal code: 8700181. ISSN: 0887-3585.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 199403

ENTRY DATE: Entered STN: 19940330

Last Updated on STN: 19940330

Entered Medline: 19940322

AB The rapid motions of the backbone of the DNA-binding domain of the glucocorticoid receptor (GR DBD) have been investigated using

proton-detected heteronuclear NMR experiments on ¹⁵N-labeled protein at pH 6.0 and with a 200 psec molecular dynamics simulation of hydrated GR DBD. The experimental data were interpreted in terms of a generalized order parameter (S₂) and an effective correlation time (tau e) for the internal motion of each amide bond. A back calculation, using the same model, yielded the [1H]-¹⁴N nuclear Overhauser effects (NOEs) and the ¹⁵N spin-lattice relaxation times (T₁) from the simulated data. The rapid motions of the backbone turned out to be rather limited and uniform throughout the protein, with a somewhat reduced mobility in the two major alpha-helical regions and a slightly enhanced flexibility for some residues in the first zinc coordinating region. The agreement between the experimental and simulated S₂-values was as good as quantitative for most of the residues, except for some residues that were subject to a more large-scale, and in the simulation thus poorly sampled, motion. Examples of such motions that were found in the simulation include jumps of the amide bond of Ile-487 between the charged oxygens of the side chain of Asp-485 and less distinct large scale motions for some of the residues in the extended regions, that were shown to give rise to noisy and/or fast decaying internal reorientational correlation functions. For these residues large differences in the simulated and experimental tau e-values were found, indicating that motions on different time scales were dominating in the experimental and simulated values. The lower (< 0.7) experimental NOEs for these residues could not be reproduced in the simulation and were shown to be a consequence of the lower tau e-values estimated in the simulation. By combining information from the simulation and the experiment a more complete picture of the motions for these residues can be obtained as is illustrated with an estimation of the jump angle and jump frequency for the amide bond of Ile-487.

CT Check Tags: Animal; Comparative Study; Support, Non-U.S. Gov't

Amino Acid Sequence

Binding Sites

*DNA: ME, metabolism

Magnetic Resonance Spectroscopy

Models, Molecular

Models, Theoretical

Molecular Sequence Data

Nitrogen Isotopes

Rats

*Receptors, Glucocorticoid: UL, ultrastructure

RN 9007-49-2 (DNA)

CN 0 (Nitrogen Isotopes); 0 (Receptors, Glucocorticoid)

L67 ANSWER 5 OF 5

MEDLINE on STN

ACCESSION NUMBER: 90234793 MEDLINE

DOCUMENT NUMBER: 90234793 PubMed ID: 2331506

TITLE: 17O- and ¹⁴N-NMR studies of Leu-enkephalin and enkephalin-related fragments in aqueous solution.

AUTHOR: Karayannis T; Gerothanassis I P; Sakarellos-Daitsiotis M; Sakarellos C; Marraud M

CORPORATE SOURCE: Department of Chemistry, University of Ioannina, Greece.

SOURCE: BIOPOLYMERS, (1990 Feb 5) 29 (2) 423-39.

Journal code: 0372525. ISSN: 0006-3525.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 199006

ENTRY DATE: Entered STN: 19900706

Last Updated on STN: 19900706

Entered Medline: 19900606

- AB 17O- and 14N-nmr chemical shifts and line widths of the carboxyl and amino terminal groups of Leu-enkephalin--Tyr-Gly-Gly-Phe-[17O]Leu-OH--and enkephalin-related fragments--[17O]Leu-OH, Phe-[17O]Leu-OH, Gly-Phe-[17O]Leu-OH, and Gly-Gly-Phe-[17O]Leu-OH--were measured in aqueous solution over the entire H pH range. Enrichment in 17O was achieved by saponification of the corresponding O-methyl esters. Ionization constants and titration shifts were obtained by nonlinear least-squares fits to one-proton titration curves. [17O]Leu-OH exhibits a profound pH-dependent solvation change on deprotonation of the carboxyl group, as shown by 17O- and 14N-nmr line widths. In contrast, the peptides studied do not exhibit pH-dependent conformational (solvation) changes on deprotonation of the carboxyl group, and a head-to-tail intramolecular association between the ionic terminal groups should be excluded. It is shown that the peptides do not exhibit isotropic overall molecular motion and that segmental motion rather than fast internal motion influences the effective correlation times at the sites of the carboxyl oxygens and the amino nitrogen.
- CT Check Tags: Comparative Study; Support, Non-U.S. Gov't
 Amino Acid Sequence
 *Enkephalin, Leucine
 Hydrogen-Ion Concentration
 Leucine
 Magnetic Resonance Spectroscopy: MT, methods
 Molecular Sequence Data
 Molecular Weight
 Nitrogen Isotopes
 Oxygen Isotopes
 *Peptide Fragments
 Protein Conformation
 Solutions
 Thermodynamics
 Water
- RN 58822-25-6 (Enkephalin, Leucine); 61-90-5 (Leucine); 7732-18-5 (Water)
 CN 0 (Nitrogen Isotopes); 0 (Oxygen Isotopes); 0 (Peptide Fragments); 0 (Solutions)

Inventor Search

WELLS 09/744,550

=> d his

(FILE 'HOME' ENTERED AT 10:19:21 ON 21 JUL 2003)

FILE 'HCAPLUS' ENTERED AT 10:19:31 ON 21 JUL 2003

L1 64 S WASHINO K?/AU
L2 37 S SHIMMURA T?/AU
L3 235 S NAKATANI A?/AU
L4 142 S FUJIMOTO C?/AU
L5 6178 S TANAKA A?/AU
L6 45 S SERI S?/AU
L7 1168 S IWAI K?/AU
L8 7854 S L1-7
L9 206 S L8 AND MAGNETIC
L10 23 S L8 AND MAGNETIC RESONANCE
L11 5768 S 170
L12 903 S 33S
L13 9485 S 14N
L14 1 S L10 AND L11-13
SELECT RN L14 1

FILE 'REGISTRY' ENTERED AT 10:22:15 ON 21 JUL 2003

L15 13 S E1-13

FILE 'HCAPLUS' ENTERED AT 10:22:38 ON 21 JUL 2003

L16 1 S L14 AND L15

1 cite of 13 cpds displayed

=> d ibib abs hitstr ind

L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:98382 HCAPLUS

DOCUMENT NUMBER: 132:134185

TITLE: Drugs for therapeutic use enabling nuclear
magnetic resonance diagnosis by
scalar bondINVENTOR(S): Washino, Komei; Shimmura, Toshiyuki
; Nakatani, Akira; Fujimoto, Chieko
; Tanaka, Akihiro; Seri, Shigemi;
Iwai, Kumiko

PATENT ASSIGNEE(S): Nihon Medi-Physics Co., Ltd., Japan

SOURCE: PCT Int. Appl., 15 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000006207	A1	20000210	WO 1999-JP3970	19990723
W: AU, BR, CA, CN, KR, NO, NZ, RU, US, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2000044491	A2	20000215	JP 1998-213050	19980728
CA 2338702	AA	20000210	CA 1999-2338702	19990723
AU 9948005	A1	20000221	AU 1999-48005	19990723
AU 758913	B2	20030403		
EP 1101498	A1	20010523	EP 1999-931523	19990723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI; LU, NL, SE, MC, PT, IE, FI				
NO 2001000423	A	20010124	NO 2001-423	20010124
PRIORITY APPLN. INFO.:			JP 1998-213050	A 19980728
			WO 1999-JP3970	W 19990723

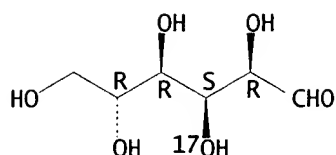
AB Drugs for therapeutic use characterized by contg. a compd. which carries in its structure at least one member selected from among -17OH, -14NH and -33SH, wherein the above 17O, 14N or 33S exerts a relaxation effect on the proton bonded thereto and the relaxation effect is transported through the exchange of a proton in a vital component of a target organ or tissue by the above-mentioned proton, thus enabling detection by NMR. The effective circulation or distribution of such a physiol. acceptable therapeutic drug in the target organ or tissue in vivo where it is needed can be externally detected by the NMR method before the administration of a remedy to each patient or simultaneously therewith.

IT 257283-87-7P, D-Glucose-3-17O 257283-88-8P, D-Glucose-1-17O
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)

RN 257283-87-7 HCAPLUS

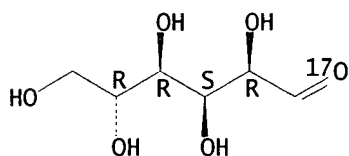
CN D-Glucose-3-17O (9CI) (CA INDEX NAME)

Absolute stereochemistry.

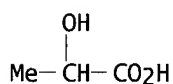


RN 257283-88-8 HCAPLUS
 CN D-Glucose-1-170 (9CI) (CA INDEX NAME)

Absolute stereochemistry.

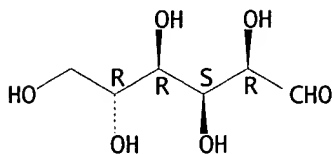


IT 50-21-5, Lactic acid, biological studies 50-99-7,
 Glucose, biological studies 4033-40-3, N-Acetyl asparagine
 7727-37-9, Nitrogen, biological studies 12586-59-3,
 Proton 13774-92-0, Imidogen 13968-48-4, biological
 studies 14257-58-0, S-33, biological studies 15587-57-2
 , Hydroxyl-170 31713-49-2, Mercapto-33S
 RL: BPR (Biological process); BSU (Biological study, unclassified); THU
 (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
 (drugs for therapeutic use enabling NMR diagnosis by scalar bond)
 RN 50-21-5 HCAPLUS
 CN Propanoic acid, 2-hydroxy- (9CI) (CA INDEX NAME)



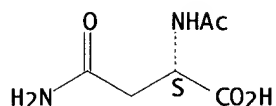
RN 50-99-7 HCAPLUS
 CN D-Glucose (8CI, 9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4033-40-3 HCAPLUS
 CN L-Asparagine, N2-acetyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 7727-37-9 HCAPLUS
CN Nitrogen (8CI, 9CI) (CA INDEX NAME)

N≡N

RN 12586-59-3 HCAPLUS
CN Proton (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 13774-92-0 HCAPLUS
CN Imidogen (8CI, 9CI) (CA INDEX NAME)

NH

RN 13968-48-4 HCAPLUS
CN Oxygen, isotope of mass 17, at. (8CI, 9CI) (CA INDEX NAME)

¹⁷O

RN 14257-58-0 HCAPLUS
CN Sulfur, isotope of mass 33 (8CI, 9CI) (CA INDEX NAME)

³³S

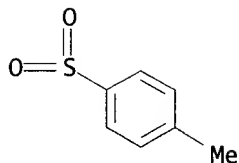
RN 15587-57-2 HCAPLUS
CN Hydroxyl-¹⁷O (7CI, 8CI, 9CI) (CA INDEX NAME)

H¹⁷O

RN 31713-49-2 HCAPLUS
CN Mercapto-³³S (8CI, 9CI) (CA INDEX NAME)

H³³S

IT **19646-38-9**, p-Toluene sulfonyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(drugs for therapeutic use enabling NMR diagnosis by scalar bond)
RN 19646-38-9 HCAPLUS
CN Phenylsulfonyl, 4-methyl- (9CI) (CA INDEX NAME)



IC ICM A61K049-00
 CC 8-9 (Radiation Biochemistry)
 Section cross-reference(s): 63
 ST radiopharmaceutical diagnosis NMR MRI scalar bond; infusion liposome
 radiopharmaceutical diagnosis NMR MRI
 IT Diagnosis
 (agents; drugs for therapeutic use enabling NMR diagnosis by scalar
 bond)
 IT Animal tissue
 Drug delivery systems
 Imaging agents
 NMR (nuclear magnetic resonance)
 Organ, animal
 Positron-emission tomography
 (drugs for therapeutic use enabling NMR diagnosis by scalar bond)
 IT Amino acids, biological studies
 RL: BPR (Biological process); BSU (Biological study, unclassified); THU
 (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
 (drugs for therapeutic use enabling NMR diagnosis by scalar bond)
 IT Drug delivery systems
 (infusions; drugs for therapeutic use enabling NMR diagnosis by scalar
 bond)
 IT Drug delivery systems
 (liposomes; drugs for therapeutic use enabling NMR diagnosis by scalar
 bond)
 IT 257283-87-7P, D-Glucose-3-170 257283-88-8P,
 D-Glucose-1-170
 RL: BPR (Biological process); BSU (Biological study, unclassified); SPN
 (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
 PREP (Preparation); PROC (Process); USES (Uses)
 (drugs for therapeutic use enabling NMR diagnosis by scalar bond)
 IT 50-21-5, Lactic acid, biological studies 50-99-7,
 Glucose, biological studies 4033-40-3, N-Acetyl asparagine
 7727-37-9, Nitrogen, biological studies 12586-59-3,
 Proton 13774-92-0, Imidogen 13968-48-4, biological
 studies 14257-58-0, S-33, biological studies 15587-57-2
 , Hydroxyl-170 31713-49-2, Mercapto-33S
 RL: BPR (Biological process); BSU (Biological study, unclassified); THU
 (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
 (drugs for therapeutic use enabling NMR diagnosis by scalar bond)
 IT 19646-38-9, p-Toluene sulfonyl
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (drugs for therapeutic use enabling NMR diagnosis by scalar bond)
 REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT